Supporting Information

Date of Preparation: October 31, 2003

Supplementary material for "Validation of Electronic Structure Methods for Hydrogen Atom Transfer Between Carbon Centers" by Agnieszka Dybala-Defratyka, Piotr Paneth, Jingzhi Pu, and Donald G. Truhlar, Journal of Physical Chemistry A.

Number of Pages: 4

TABLE S1. Root Mean Squared Error (RMSE in kcal/mol) for Methods Over the Representative Data Set[a]

Method	BH6	BH4	AE6[b]	AE3[b]
***N*[7]**				
G3S//MP2(full)/6-31G(d)[c]	0.45	0.53	0.54	0.50
G3SX(MP3)//B3LYP/6-31G(2df,p)	0.40	0.39	0.39	0.36
CBS-APNO//QCISD/6-311G(d,p)	n.a.[d]	1.42	n.a.	0.49
CBS-QB3//B3LYP/6-31G(d[†])	0.76	0.87	0.80	0.57
MCG3/3	n.c.[e]	n.c.	n.c.	n.c.
MCG3/3//MPW1K/6-31+G(d,p)	0.92	0.64	0.59	0.26
CBS-Q//MP2/6-31G(d[†])	0.93	1.09	0.80	0.62
***N*[6]**				
MC-QCISD/3//MPW1K/6-31+G(d,p)	0.82	0.70	0.59	0.26
MC-QCISD/3	1.00	0.94	n.c.	n.c.
CBS-4M//UHF/3-21G(d)	2.95	3.59	1.36	1.18
***N*[5]**				
SAC/3	3.49	3.96	3.96	3.03
MP2/6-31+G(d,p)	5.68	5.91	12.18	12.14
MP2/6-31G(d)	7.42	7.58	18.52	20.40
***N*[4]**				
MPW1K/MG3S	1.52	1.60	5.55	4.83
MPW1K/6-31+G(d,p)	1.74	2.05	7.68	6.20
MPW1K/MG3S//MPW1K/6-31+G(d,p)	1.53	1.61	5.62	4.88
MPW1K/MIDIY+	2.30	2.56	13.22	14.07
MPW1K/6-31G(d)	3.44	4.20	7.59	5.85
B3LYP/6-31+G(d,p)	5.60	6.58	3.34	2.50
HF/MIDI!	14.15	16.46	89.73	97.35
HF/6-31+G(d,p)	14.62	16.35	77.08	82.42
HF/6-31G(d)	15.58	17.51	77.61	82.84

***N*³**				
PM3-3H2	3.63	3.74	10.07	10.63
AM1	6.24	6.88	13.49	11.60
PM3	5.74	4.81	10.07	10.63
AM1-CHC-SRP	7.15	8.50	13.76	14.19
PM3-NHR	6.92	6.74	10.09	10.65
PM3-AHR	8.77	9.06	1.89	13.94
PM3-CHC-SRP	8.95	9.11	13.39	14.38
PM3tm	9.10	9.89	11.81	10.64
SAM1	13.89	7.04	20.19	6.95
MSINDO	10.85	9.75	2.18	2.26
PM5	14.19	5.73	10.41	10.55
MNDO	21.66	25.70	8.48	9.39
MNDO/d	22.05	25.70	14.04	9.36
PDDG/PM3	n.a.	8.74	n.a.	8.39
PDDG/MNDO	n.a.	25.22	n.a.	37.18
MNDOC	n.a.	24.73	n.a.	1.64

[a]See Ref. 48 and http://comp.chem.umn.edu/database/
[b]in kcal/mol per bond (counting double bonds and triple bonds as a single bond). Molecules in AE6 and AE3 contain 29 and 23 bonds respectively.
[c]X//Y denotes a single-point calculation by method X at geometry optimized by method Y. When no // is present, X and Y are the same.
[d]n.a. denotes that the method is not available for second row elements.
[e]n.c. denotes not calculated.

TABLE S2. Mean Signed Error (MSE in kcal/mol) for Methods Over the Representative Data Set[a]

Method	BH6	BH4	AE6[b]	AE3[b]
***N*[7]**				
G3S//MP2(full)/6-31G(d)[c]	0.04	-0.03	-0.08	-0.01
G3SX(MP3)//B3LYP/6-31G(2df,p)	-0.14	-0.01	0.08	0.09
CBS-APNO//QCISD/6-311G(d,p)	n.a.[d]	-1.12	n.a.	0.16
CBS-QB3//B3LYP/6-31G(d†)	-0.49	-0.61	0.16	-0.03
MCG3/3	n.c.[e]	n.c.	n.c.	n.c.
MCG3/3//MPW1K/6-31+G(d,p)	0.49	0.13	0.01	0.01
CBS-Q//MP2/6-31G(d†)	-0.56	-0.70	0.17	-0.02
***N*[6]**				
MC-QCISD/3//MPW1K/6-31+G(d,p)	0.58	0.39	-0.09	-0.01
MC-QCISD/3	0.84	0.72	n.c.	n.c.
CBS-4M//UHF/3-21G(d)	-1.96	-3.19	0.53	0.34
***N*[5]**				
SAC/3	3.08	3.60	0.02	0.51
MP2/6-31+G(d,p)	5.00	5.80	-4.85	-4.09
MP2/6-31G(d)	7.00	6.98	-6.36	-6.74
***N*[4]**				
MPW1K/MG3S	-1.21	-1.20	-2.08	-1.54
MPW1K/6-31+G(d,p)	-1.12	-1.34	-2.95	-1.89
MPW1K/MG3S//MPW1K/6-31+G(d,p)	-1.21	-1.20	-2.11	-1.56
MPW1K/MIDIY+	-1.92	-2.04	-5.03	-4.94
MPW1K/6-31G(d)	-0.60	-0.92	-2.98	-1.79
B3LYP/6-31+G(d,p)	-4.71	-6.43	-1.30	-0.90
HF/MIDI!	11.03	12.72	-34.71	-34.55
HF/6-31+G(d,p)	13.40	14.99	-30.74	-29.33
HF/6-31G(d)	13.73	15.25	-31.04	-29.48
***N*[3]**				
PM3-3H2	1.48	2.99	-2.94	-3.16
AM1	2.39	4.63	-4.85	-3.67
PM3	1.68	1.04	-2.94	-3.16
AM1-CHC-SRP	3.61	5.77	-5.29	-4.11
PM3-NHR	2.81	2.71	-2.94	-3.16
PM3-AHR	3.53	3.83	-3.72	-4.14
PM3-CHC-SRP	3.89	4.15	-3.88	-4.24
PM3tm	4.44	5.13	-4.22	-3.16
SAM1	-9.47	-5.56	-3.64	-0.51
MSINDO	10.42	9.33	0.67	0.62
PM5	-7.89	-0.37	-3.87	-3.20

MNDO	17.83	24.81	-2.76	-2.99
MNDO/d	20.44	24.81	0.86	-2.98
PDDG/PM3	n.a.	-4.67	n.a.	0.26
PDDG/MNDO	n.a.	23.79	n.a.	-13.22
MNDOC	n.a.	24.41	n.a.	-0.16

[a]See Ref. 48 and http://comp.chem.umn.edu/database/
[b]in kcal/mol per bond (counting double bonds and triple bonds as a single bond). Molecules in AE6 and AE3 contain 29 and 23 bonds respectively.
[c]X//Y denotes a single-point calculation by method X at geometry optimized by method Y. When no // is present, X and Y are the same.
[d]n.a. denotes that the method is not available for second row elements.
[e]n.c. denotes not calculated.